Generative Deep Neural Networks for Inverse Materials Design Using Backpropagation and Active Learning

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Abstract

In recent years, machine learning (ML) techniques are seen to be promising tools to discover and design novel materials. However, the lack of robust inverse design approaches to identify promising candidate materials without exploring the entire design space causes a fundamental bottleneck. A general■purpose inverse design approach is presented using generative inverse design networks. This ML■based inverse design approach uses backpropagation to calculate the analytical gradients of an objective function with respect to design variables. This inverse design approach is capable of overcoming local minima traps by using backpropagation to provide rapid calculations of gradient information and running millions of optimizations with different initial values. Furthermore, an active learning strategy is adopted in the inverse design approach to improve the performance of candidate materials and reduce the amount of training data needed to do so. Compared to passive learning, the active learning strategy is capable of generating better designs and reducing the amount of training data by at least an order■of■magnitude in the case study on composite materials. The inverse design approach is compared with conventional gradient■based topology optimization and gradient■free genetic algorithms and the pros and cons of each method are discussed when applied to materials discovery and design problems.